

Scale-renormalized matrix-product states for correlated quantum systems

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A generalization of matrix product states (MPS) is introduced which is suitable for describing interacting quantum systems in two and three dimensions. These *scale-renormalized matrix-product states* (SR-MPS) are based on a coarse-graining of the lattice in which the blocks at each level are associated with matrix products that are further transformed (scale renormalized) with other matrices before they are assembled to form blocks at the next level. Using variational Monte Carlo simulations of the two-dimensional transverse-field Ising model as a test, it is shown that the SR-MPS converge much more rapidly with the matrix size than a standard MPS. It is also shown that the use of lattice-symmetries speeds up the convergence very significantly.

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In a variational study of an interacting quantum system, a wave function Ψ with a number of adjustable parameters p_1, \dots, p_m is optimized by minimizing its energy $E = \langle \Psi | H | \Psi \rangle$ with respect to a hamiltonian H . Ideally, one would like to consider a functional form which allows for a systematic way of improving the calculation, by increasing the number of parameters m in such a way that Ψ is guaranteed to approach the true ground state of H in the limit $m \rightarrow \infty$. A trivial way, in principle, is to expand $|\Psi\rangle$ in a complete set of states; $|\Psi\rangle = \sum_n c_n |n\rangle$, whence the parameters to be optimized are the wave function coefficients c_n themselves. However, in practice, the Hilbert space is too large (2^N states in the simplest case of N spins with $S = 1/2$) to include all states, and in general there is no obvious way to order the states so that their contributions to the ground state decrease as a function of n . To achieve this, one can attempt to optimize the basis in some way, with the goal of obtaining a hierarchy of basis states which systematically and rapidly improve the result as they are included in the calculation. This is the basic idea of renormalization group (RG) methods, which after decades of attempts, following Wilson's pioneering solution of Kondo impurity problem [1], led to a break-through in the form of White's density matrix RG (DMRG) method [2, 3] for one-dimensional systems.

For systems in higher dimensions, there has been recent progress in generalizing the DMRG approach, which is closely related to matrix-product states (MPS) [4], using tensor-network states [5], e.g., the projected entangled pair states (PEPS) [6] and related MPS-like string states [7], as well as schemes based on entanglement renormalization [8]. However, there are still considerable challenges related to the convergence properties and computational complexity of these methods. In this Letter, an alternative class of generic correlated states—*scale-renormalized matrix-product states* (SR-MPS)—is introduced. These states combine concepts of coarse graining, renormalization, and MPS into a framework for systematically refined variational calculations. The

scheme is tested on the two-dimensional transverse-field Ising model, using a recently developed variational Monte Carlo method [9] to optimize the SR-MPS.

In the DMRG method, the basis is re-optimized and truncated at some number D of states as more sites are added to the lattice [2]. Originally this was not viewed as a variational method, but it was soon recognized that the DMRG in effect produces the best variational MPS with $D \times D$ matrices [4]. For a system of N spins represented by Pauli operators $\vec{\sigma}_i$, and working in the basis where all σ_i^z are diagonal, $\sigma_i^z = \pm 1$, MPS for a periodic chain are of the form (using the notation $[\sigma]$ for $[\sigma_1^z, \dots, \sigma_N^z]$)

$$|\Psi\rangle = \sum_{[\sigma^z]} W([\sigma]) |\sigma_1^z, \dots, \sigma_N^z\rangle, \quad (1)$$

where the wave-function coefficient is

$$W([\sigma]) = \text{Tr}\{A(\sigma_1^z)A(\sigma_2^z) \cdots A(\sigma_N^z)\}, \quad (2)$$

and $A(\pm 1)$ are two $D \times D$ matrices. For systems with open boundaries, for which DMRG and standard MPS techniques are best suited in practice, the matrices are site dependent, and instead of taking a trace the edge matrices are vectors. The DMRG method does not operate with MPS explicitly, but recently schemes have been devised for working directly with the MPS without invoking the DMRG procedures. This formally reduces the scaling of the computational effort from D^6 to D^5 for periodic systems [10]. Using Monte Carlo sampling of the spins states, instead of evaluating their traces exactly, the scaling can be further reduced to D^3 [7, 9].

In higher dimensions, the DMRG method typically is implemented by regarding the system as a chain folded up to form the lattice of interest [11]. In this effective one-dimensional system there are long-range interactions. Further studies of the MPS formalism also showed why the DMRG method performs poorly in this case. The exponential scaling in the number of states that has to be kept [12], or, equivalently, the matrix dimension D of the MPS, is a consequence of the inability of the matrix

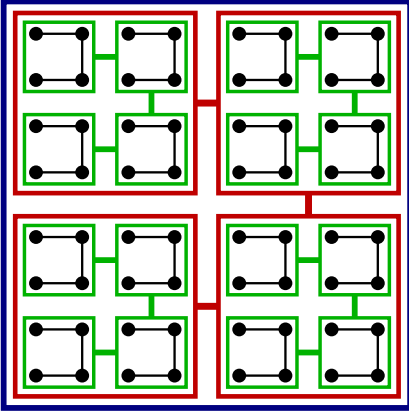


FIG. 1: (Color online) SR-MPS hierarchy for a square lattice. The circles represent the original matrices $B_{x,y}^0 = A(\sigma_{x,y})$. Products of four of these are indicated by connecting lines. A square enclosing such a unit represents scale renormalization with matrices M_L^n, M_R^n , which results in $B_{x,y}^1$. Successive levels of connected squares enclosed by larger squares represent products of four matrices $B_{x,y}^n$ followed by scale renormalizations with M_L^n, M_R^n , resulting in $B_{x,y}^{n+1}$.

products to account for entanglement between neighboring sites when the corresponding matrices are far apart [13]. To circumvent this problem, tensor-network states have been proposed as natural and effective generalizations of the MPS/DMRG to higher dimensions [5, 6].

Here SR-MPS is proposed as an alternative generalization of MPS for higher-dimensional systems. For a periodic system of $S = 1/2$ spins $\vec{\sigma}_{x,y}$, each lattice site (x, y) , $x, y = 1, \dots, L$, is associated with a $D \times D$ matrix $A(\sigma_{x,y}^z)$ as in the MPS. However, instead of just arranging these matrices according to a string on the lattice, the system is first subdivided into blocks, which are associated with matrix products. These matrix products are then *scale renormalized* by transforming them with some other matrices, before they are multiplied by similar block-matrices to represent a larger cell. For a square lattice, the resulting hierarchy of matrix products (in the simplest case based on blocks with four sub-blocks at each level) is illustrated in Fig. 1. The block-matrices at levels n and $n+1$ are related according to

$$B_{x,y}^{n+1} = M_L^n B_{x,y}^n B_{x+1,y}^n B_{x+1,y+1}^n B_{x,y+1}^n M_R^n, \quad (3)$$

with the lowest level corresponding to the original spin dependent matrices, $B_{x,y}^0 = A(\sigma_{x,y}^z)$, and M_L^n, M_R^n accomplishing the scale renormalization. At level n the block coordinates take the values $k2^n$, $k = 1, \dots, L/2^n$. Thus the lattice size should be a power of 2; $L = 2^l$.

The purpose of the scale renormalization is to compensate, as much as possible, for the non-equivalent ways in which the four blocks at a given level n are treated in the associated product of four matrices. It will be shown that the effect indeed is to make the four members of a block more uniform in their correlations with each other and the rest of the system.

Note that under the trace of the final assembly of products, $B_{1,1}^l$, an equivalent way of defining the block matrices (3) is with a single scale-renormalization matrix; $B_{x,y}^{n+1} = B_{x,y}^n B_{x+1,y}^n B_{x+1,y+1}^n B_{x,y+1}^n M^n$. However, Eq. (3) allows for the possibility of increasing the matrix size with the level n , using rectangular matrices M_L^n and M_R^n of size $D_{n+1} \times D_n$, and $D_n \times D_{n+1}$, respectively. This may be useful if the scale-renormalization is further refined by making $M_{L,R}^n$ dependent on the physical state of the blocks they transform, using, e.g., a block spin $\Sigma_{x,y} = 0, \pm 1$ [for six different matrices $M_{L,R}^n(\Sigma_{x,y})$]. Defining an appropriate block-variable for a given model is not always easy, however. In the Ising model considered here the Kadanov block-spin [14] can be used, but in this first study only the state-independent scale-renormalization (3) will be applied and the matrix size will be kept constant; $D_n = D$. Keeping the symmetric form with left and right scale-renormalizations, instead of just a single M^n , seems to help in the optimization, in spite of the larger number parameters.

In the simplest version of the SR-MPS the wave function coefficient is the trace of $B^l \equiv B_{1,1}^l$. One can also use a sum of matrix products taken over symmetry transformations of the spin configuration. Spin-inversion symmetry can be used if the hamiltonian has it. Then

$$W([\sigma]) = \text{Tr}\{B^l([\sigma]) \pm B^l(-[\sigma])\}, \quad (4)$$

where $-[\sigma]$ denotes the configuration with all $\sigma_i \rightarrow -\sigma_i$. It is also useful to incorporate lattice symmetries. Denoting a transformation (including the identity) of $[\sigma]$ (translation, rotation, or reflection) by $T_r[\sigma]$, the wave function coefficient is, considering for simplicity a fully symmetric wave function with zero momentum,

$$W([\sigma]) = \sum_r \text{Tr}\{B^l(T_r[\sigma]) + B^l(-T_r[\sigma])\}. \quad (5)$$

Here $r = 1, \dots, 8N$ if all symmetries of the square lattice are used. It will be shown below that the use of symmetries improves the D convergence very significantly.

To test the SR-MPS scheme, it will be applied next to the Ising model in a transverse field;

$$H = - \sum_{x,y} (\sigma_{x,y}^z \sigma_{x+1,y}^z + \sigma_{x,y}^z \sigma_{x,y+1}^z + h \sigma_{x,y}^x), \quad (6)$$

with periodic boundaries ($\sigma_{L+1,y}^z = \sigma_{1,y}^z$ and $\sigma_{x,L+1}^z = \sigma_{x,1}^z$). Computations are expected to be the most challenging at quantum-critical points; h in the vicinity of $h_c \approx 3.044$ [15] will be the main focus here.

To optimize the wave function, here using general (non-symmetric) real matrices $A(\pm 1)$ and M_L^n, M_R^n , $n = 1, \dots, l$, the variational Monte Carlo method discussed in Ref. [9] is used. The energy derivatives are calculated, and based on their signs the matrix elements are updated by a random amount, e.g., $a_{ij} \rightarrow a_{ij} - \text{sign}(\partial E / \partial a_{ij}) \delta r_{ij}$. Here $r_{ij} \in [0, 1)$ is a random number and the maximum

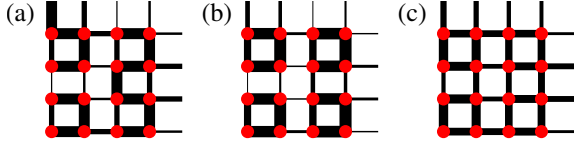


FIG. 2: (Color online) Nearest-neighbor spin correlations on a 4×4 lattice at $h = 3$ calculated using (a) an MPS with $D = 2$, (b) an SR-MPS with $D = 2$, and (c) an SR-MPS with $D = 8$. The thinnest and thickest bars correspond, respectively, to a -11% and $+11\%$ deviation from the average. The bars at the right and upper edges represent the correlations across the boundaries (periodic boundary conditions are used). The energies $-E/N$ of the states in (a),(b),(c) are 3.1746, 3.1772, 3.2108. The exact energy for $L = 4$ is -3.2155081 .

step δ is gradually reduced. If this reduction is sufficiently slow, the converged matrices will correspond to an energy minimum. Calculations in one-dimension [9] have shown that the global energy minimum, which evolves to the true ground-state energy with increasing D , can be reached with this method at least up to $D \approx 50$.

If no lattice symmetries are used, the Metropolis probability of flipping a spin can be evaluated with $\propto D^3$ operations using the sequential flip scheme of Ref. [9]. However, with symmetries incorporated according to Eq. (5), the spins cannot be sequentially visited in all transformed configurations, and therefore a different scheme has to be employed. Organizing partial products in tree-structures, one for each lattice transformation, the total number of operations required for each spin update is $\propto N \ln(N) D^3$, where the factor N is due to the number of different matrix products and $\ln(N)$ comes from recalculating one branch of a tree.

First, an $L = 4$ lattice will be considered. To demonstrate some of the effects of scale-renormalization, Fig. 2 shows a plot of the spatial variations in the nearest-neighbor correlations $\langle \sigma_{x,y}^z \sigma_{x+1,y}^z \rangle$ and $\langle \sigma_{x,y}^z \sigma_{x,y+1}^z \rangle$, obtained with and without scale-renormalization. Spin-inversion symmetry is taken into account but no lattice symmetries are used, i.e., the states are sampled according to the symmetric (+) Eq. (4). With a small D one would then expect to see traces of the particular way the blocks are constructed. Without scale-renormalization (i.e., $M_L^n, M_R^n = I$), the scheme reduces to an MPS calculation with the matrix product taken along the particular “coarse-graining string” used here in the SR-MPS. In Fig. 2(a), obtained with $D = 2$, it can be seen clearly that the correlations are non-uniform; in particular different sites within the 2×2 blocks are not equally correlated with their neighbors. With scale-renormalization, Fig. 2(b) shows a significantly reduced non-uniformity between the blocks. The energy is also improved. With $D = 8$ in the SR-MPS, shown in Fig. 2(c), the non-uniformity is much reduced and the energy is improved considerably. In contrast, an MPS with $D = 8$ (not shown) only marginally improves on the $D = 2$ result.

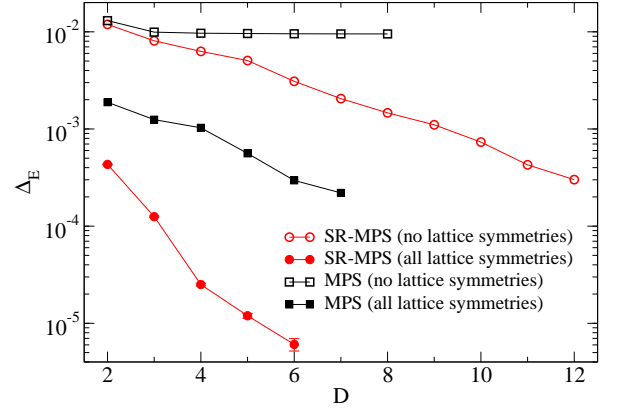


FIG. 3: (Color online) Relative deviation $\Delta_E = (E - E_D)/E$ of the energy E_D of SR-MPS and MPS with $D \times D$ matrices from the exact energy E for a 4×4 system at $h = 3$.

Fig. 3 illustrates the convergence of MPS and SR-MPS with and without lattice symmetries. Without lattice symmetries, the MPS energy converges extremely slowly and it is not possible in practice to obtain the ground state. By incorporating the lattice symmetries the convergence is substantially improved, however. In the case of the SR-MPS, an exponential convergence with D is seen even without lattice symmetries, and with these symmetries included the convergence is very rapid, with an accuracy of 10^{-5} reached already at $D = 5$. Clearly, both lattice symmetries and scale renormalization have very favorable effects, and when using both of them the convergence properties seem very encouraging.

Before moving to larger lattices, a further improvement of the SR-MPS is noted: One can use different matrices for all the states of a block of spins, instead of just the two matrices $A(\sigma_{x,y}^z)$ for individual spins. Using 2×2 blocks, there are 16 matrices $A(\sigma_{x,y}^4)$, where $\sigma_{x,y}^4 = 0, \dots, 15$ labels the states of the spins $\sigma_{x,y}^z, \sigma_{x+1,y}^z, \sigma_{x,y+1}^z, \sigma_{x+1,y+1}^z$. This gives additional flexibility to the wave function, and thus a faster D convergence can be expected. The larger number of matrices to optimize does not seem to pose any difficulties in practice, and in addition roughly four times less operations are required for a spin update. Here calculations with 2×2 -block matrices $A(0, \dots, 15)$, will be compared with the basic $A(\pm 1)$ scheme.

Fig. 4 shows the D convergence of the energy and the magnetization of an 8×8 lattice close to the quantum-critical point; $h = 3.044$. Results for comparison, $E/N = -3.23627(2)$ and $m^2 = 0.14073(1)$, were obtained with the stochastic series expansion (SSE) method [16]. Again it can be seen that the use of lattice symmetries is crucial for achieving good convergence. The convergence is also significantly better with the block matrices $A(0, \dots, 15)$ than with single-spins matrices $A(\pm 1)$.

As with MPS or PEPS the accuracy of an SR-MPS calculation with fixed D is expected to be lowest at a quantum-critical point. This is explicitly demonstrated

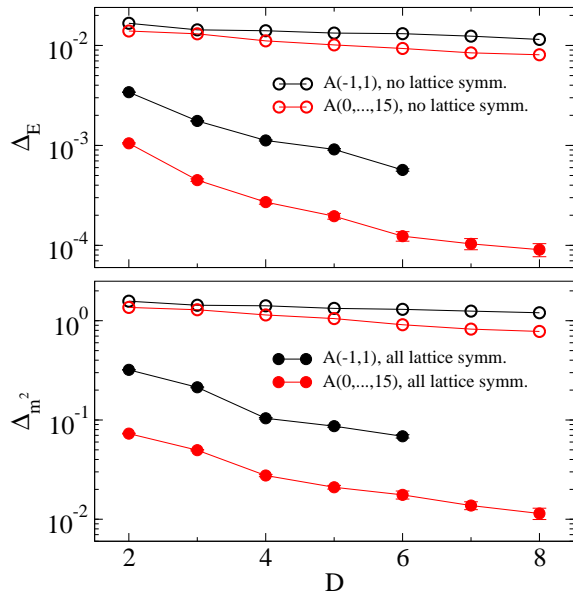


FIG. 4: (Color online) Relative error of the energy and the squared magnetization for an $L = 8$ system at $h = 3.044$, using SR-MPS with single-spin $A(\pm 1)$ matrices and 2×2 block matrices $A(0, \dots, 15)$, with and without lattice symmetries.

for the SR-MPS description of the transverse-field Ising model in Fig. 5, using both single-spin and 2×2 block matrices with $D = 4$. With the single-spin matrices, the error in the squared magnetization in the neighborhood of the critical field is $\approx 10\%$, and with the 2×2 block matrices it is $\approx 3\%$. The accuracy of the SR-MPS increases rapidly away from the critical point.

In Ref. [7] string-state calculations for a 10×10 lattice were reported. A magnetization curve exhibiting a phase transition was obtained, but the accuracy is actually rather poor close to the critical point, with deviations of more than 50% from the exact result and too little finite-size rounding. Since no systematic convergence tests were presented it is difficult to compare the performance of SR-MPS and string states directly.

Although the 8×8 lattice considered here is small in the context of QMC simulations of sign-problem-free models, the calculations demonstrate that the SR-MPS approach is a practically feasible. One important question is of course how the D required to obtain a desired accuracy grows as N increases. In order for the scaling to be a power-law, instead of exponential, it is believed that an area law for the entanglement entropy has to be obeyed [17]. Because of the lattice symmetries incorporated, the SR-MPS may satisfy such a law [18]. This, however, would still not guarantee a power-law scaling. Numerically it is also currently difficult to establish the scaling, because a range of system sizes are needed. Calculations for $L = 16$ at $h = h_c$ give an energy error $\Delta_E < 0.2\%$ for $D = 5$. Thus it is at least clear that one can access practically useful lattice sizes.

The SR-MPS scheme also work for frustrated systems.

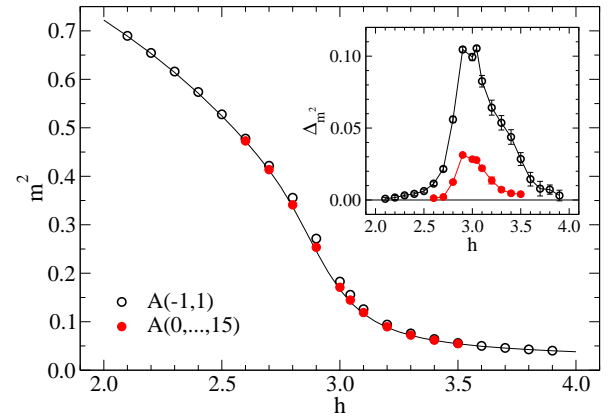


FIG. 5: (Color online) Squared magnetization as a function of the external field for an $L = 8$ system obtained with $D = 4$ SR-MPS, using matrices either for single spins or for blocks of 2×2 spins at the lowest level. The solid curve shows results obtained with the approximation-free SSE method. Relative errors are shown in the inset.

Preliminary calculations for an $L = 8$ square-lattice $S = 1/2$ Heisenberg model with a ratio $J_2/J_1 = 0.5$ of the second-nearest to nearest-neighbor interaction show a slower convergence with D than in Fig. 4, but it does appear feasible to reach the ground state.

It was shown here that incorporation of lattice symmetries in the wave function is crucial for achieving good convergence. This has also been noted for one dimensional MPS [19]. Although the scaling of the computation increases by a factor of N , to $\propto D^3 N^2 \ln(N)$ operations for updating the whole system, this can be partially alleviated by parallelizing the calculation of the spin-flip probability—the $8N$ different traces can be calculated completely independently of each other.

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- [1] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1995).
 - [2] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
 - [3] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).
 - [4] S. Östlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995).
 - [5] T. Nishino *et al.*, Nucl. Phys. B **575**, 504 (2000).
 - [6] F. Verstraete and J. I. Cirac, Arxiv:cond-mat/0407066.
 - [7] N. Schuch, M. M. Wolf, F. Verstraete, and J. I. Cirac, arXiv:0708.1567.
 - [8] G. Vidal, ArXiv:cond-mat/0512165.
 - [9] A. W. Sandvik and G. Vidal, arXiv:0708.2232 (to appear in Phys. Rev. Lett.).
 - [10] F. Verstraete, D. Porras, J. I. Cirac, Phys. Rev. Lett. **93**, 227205 (2004).
 - [11] S. R. White and D. J. Scalapino, Phys. Rev. Lett. **91**, 136403 (2003).

- [12] S. Liang and H. Pang, Phys. Rev. B **49**, 9214 (1994).
- [13] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).
- [14] L. P. Kadanov, Physics **2**, 263 (1966).
- [15] H. Rieger and N. Kawashima, Eur. Phys. J. B **9**, 233 (1999).
- [16] A. W. Sandvik, Phys. Rev. E **68**, 056701 (2003).
- [17] F. Verstraete, M. M. Wolf, D. Perez-Garcia, and J. I. Cirac, Phys. Rev. Lett. **96**, 220601 (2006).
- [18] G. Vidal (private communication).
- [19] D. Porras, F. Verstraete, and J. I. Cirac, Phys. Rev. B **73**, 014410 (2006).